Article

Using Isopropanol as a Capping Agent in the Hydrothermal Liquefaction of Kraft Lignin in Near-Critical Water

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Table S1. Average temperature and pressure, and their respective ranges, during the reaction. Calculated with $\Psi_{avg} = \int_{t_1}^{t_2} \Psi(t)dt\,/(t_2 - t_1)$ where t_2 is the time of discharge from the reactor, t_1 is the time when the injection was completed and Ψ is either the temperature or pressure. Yields of product fractions and the amount of IPA added remaining in the reactor product measured with gas chromatography with flame ionisation detector (PerkinElmer GC-FID, Clarus 690; PerkinElmer Life and Analytical Sciences, Shelton, CT, USA). The GC-FID program started at 85°C for 1 min followed by a 20°C/min heating rate to 160°C and a final hold at that temperature for 2 minutes. The column used was an Elite BAC-1 PE N9315071 and an internal standard of 1-propanol was used.

IPA/Dry lignin [g/g]	Nominal T [°C]	T_{avg} [°C]	T range [°C]	P_{avg} [bar]	P range [bar]	Char yield [%]	Precipitated solids yield [%]	ASO yield [%]	IPA remaining [%]
IPA Series									
0	320	313	283-317	250	174-265	36	19	16	--
0.6	320	314	272-317	248	185-261	31	27	13	67
2.7	320	321	303-324	247	236-262	20	33	15	71
4.9	320	314	279-318	243	181-259	27	36	20	82
Ref.	320	319	291-323	242	184-257	--	--	--	73
Temperature Series									
2.7	290	293	252-297	256	190-263	16	46	22	85
2.7	320	321	303-324	247	236-262	20	33	15	71
2.7	335	334	315-336	248	224-257	27	29	23	71

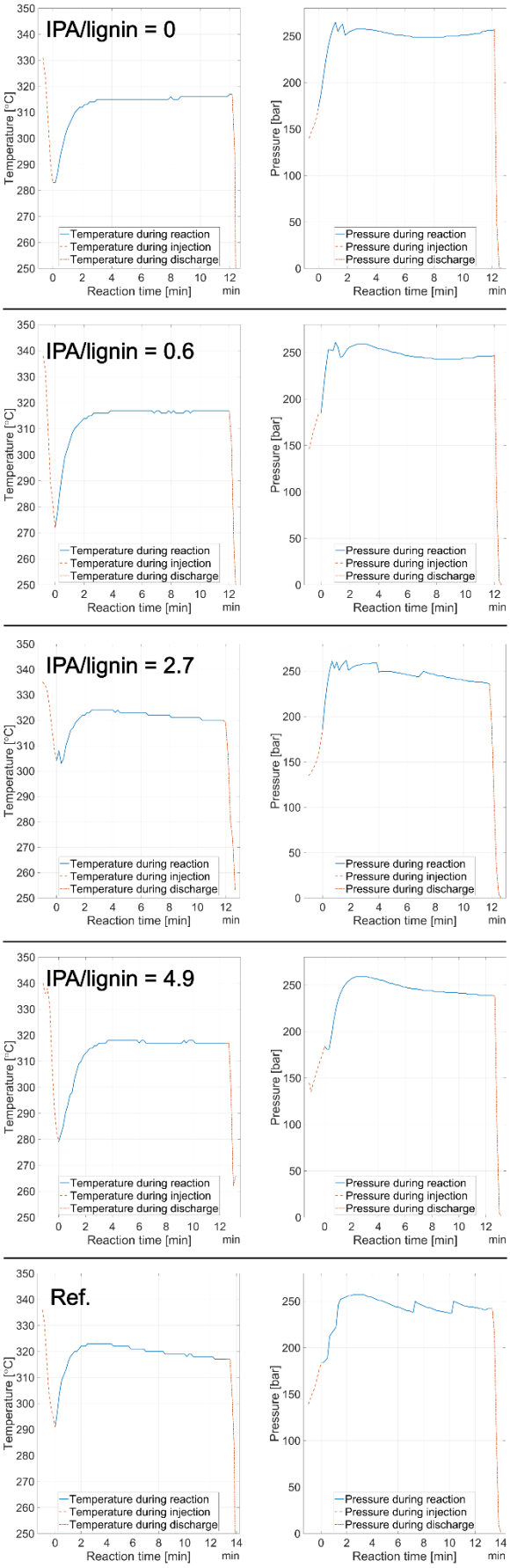

Figure S1. Temperature (left) and pressure (right) profiles in the reactor during injection, reaction, and discharge in the IPA series.

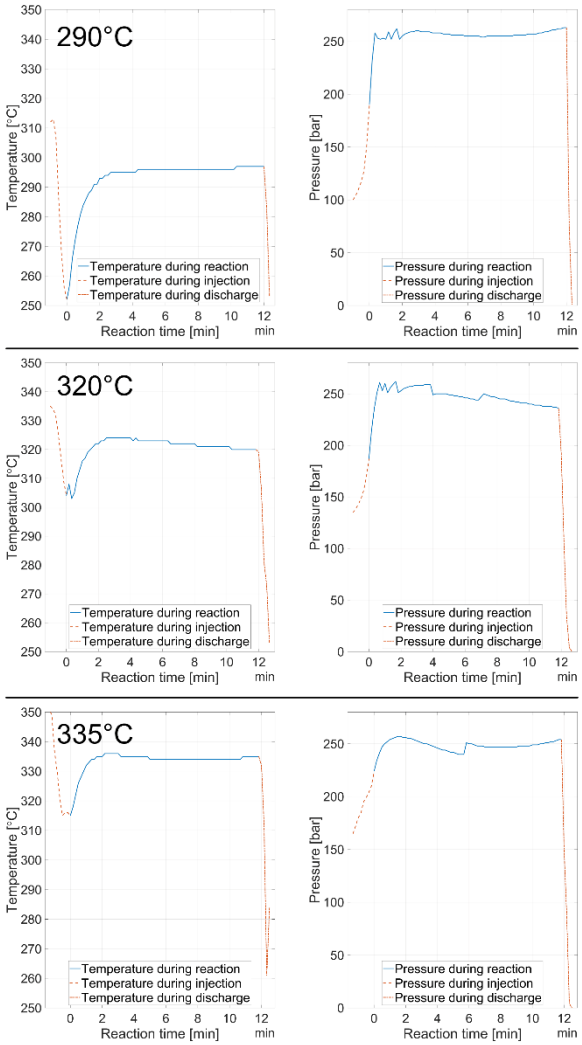

Figure S2. Temperature (left) and pressure (right) profiles in the reactor during injection, reaction, and discharge in the temperature series.

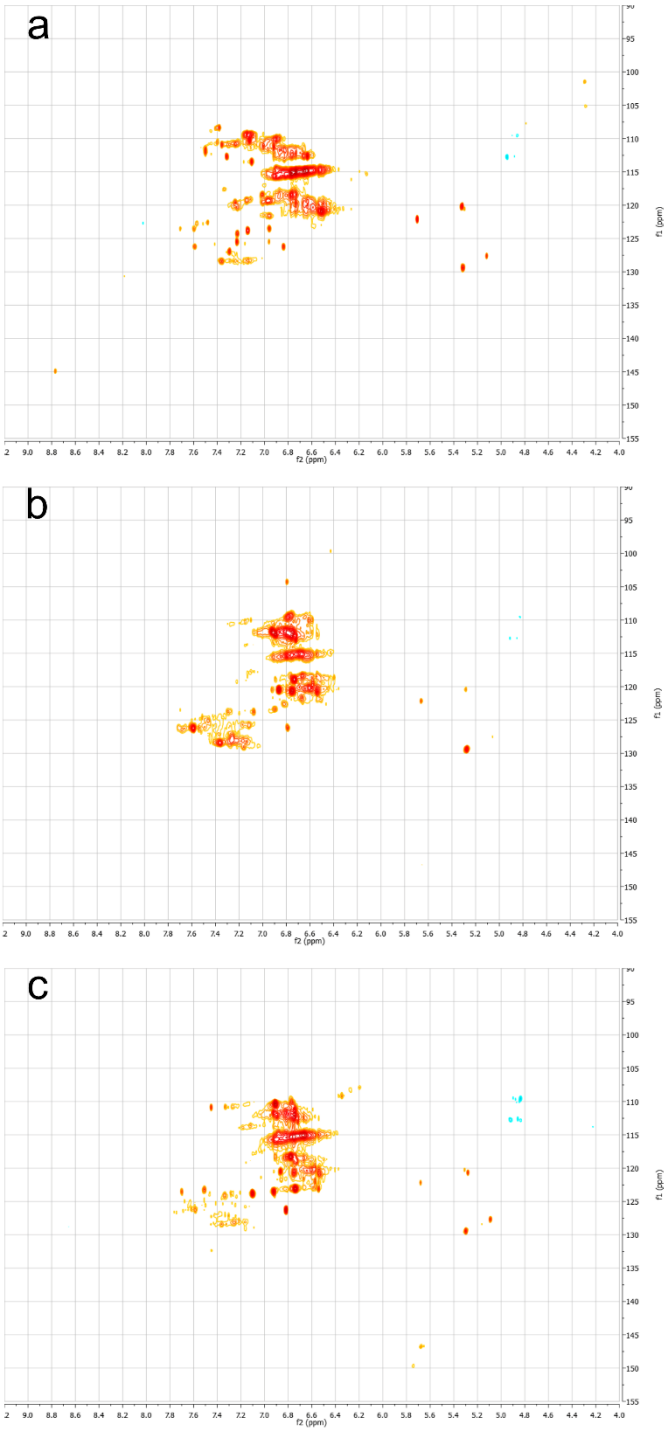

Figure S3. Aromatic region, δ_C/δ_H 90-155/4.0-9.2ppm, of the heteronuclear single quantum coherence spectroscopy (HSQC) spectra of the LignoBoost lignin (a), char (b) and precipitated solids (c).

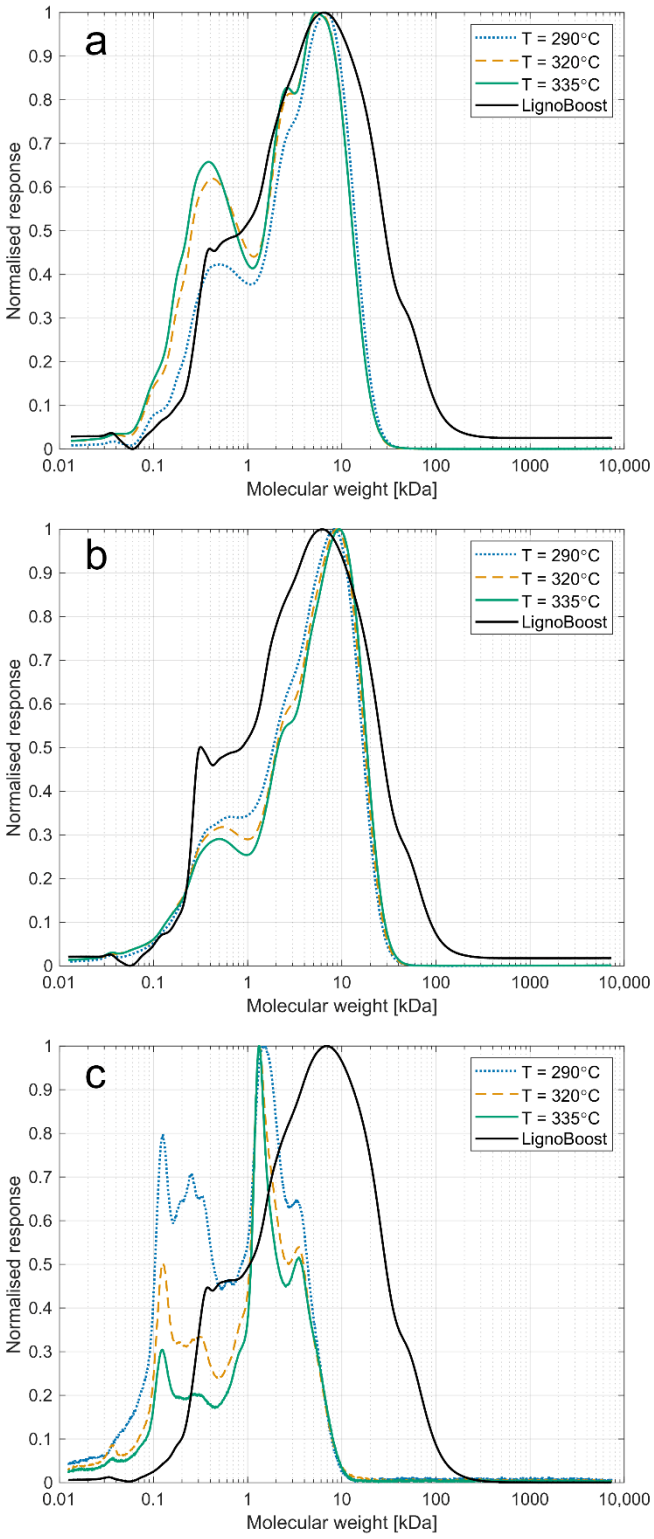

Figure S4. Gel permeation chromatography (GPC) chromatograms in the temperature series for char (a), precipitated solids (b) and ASO (c).

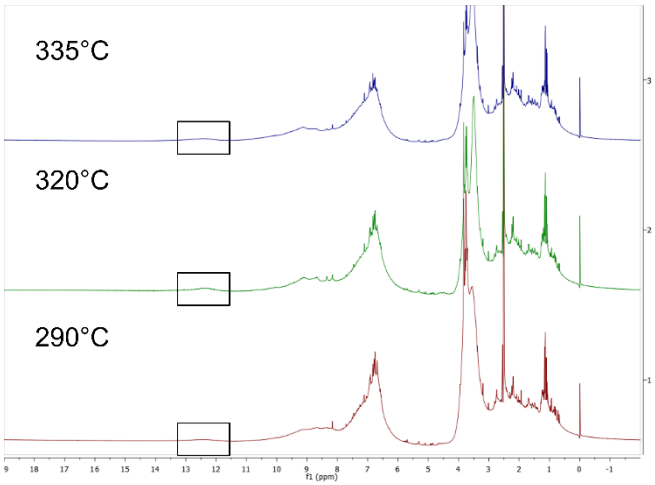

Figure S5. ^{1}H-NMR spectra of the precipitated solids in the temperature series: 335°C, 320°C and 290°C. The weak broad peak between 12 and 13 ppm in each spectrum, marked with a black box, represents the carboxylic acids.

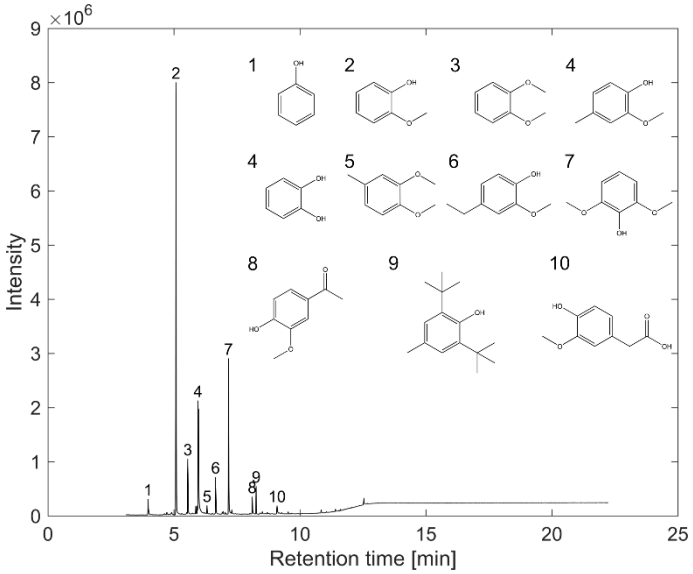

Figure S6. Typical gas chromatography (GC) chromatogram of the DEE-extracted ASO. Peak 4 is a mixture of creosol and catechol and therefore not properly resolved, Peak 7 is the internal standard and Peak 9 the solvent preservative.